

# Volume Reflection and Volume Refraction of Relativistic Particles in a Uniformly Bent Crystal \*

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The scattering of fast charged particles in a bent crystal has been analyzed in the framework of relativistic classical mechanics. The expressions obtained for the deflection function are in satisfactory agreement with the experimental data for the volume reflection of relativistic protons obtained in [1,2,3]. The features of the scattering of the particles on ring potentials are considered in a wide range of impact parameters.

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In the 1980s, studying the effect of the volume capture of relativistic protons into the channeling regime, Taratin and Vorobiev [4, 5] demonstrated the possibility of volume reflection, i.e., the coherent small-angle scattering of particles at angle  $\theta \lesssim 2\theta_L$  ( $\theta_L$  is the Lindhard critical angle) to the side opposite to the bending of the crystal. Recent experiments reported in [13] confirm the presence of this effect for 1-, 70-, and 400-GeV proton beams in a Si crystal. The conclusions made in [4, 5] were based primarily on the numerical simulation. In view of this circumstance, the aim of this work is to derive analytical expressions for the deflection function of relativistic particles. At first sight, the perturbation theory in the potential can be applied at relativistic energies and weak crystal potential [ $U(r) \approx 10 - 100$ ]. However, the relativistic generalization of the known classical formula for small-angle scattering in the central field [6],

$$\chi = -b \int_b^\infty \frac{d\phi}{dr} \frac{dr}{\sqrt{r^2 - b^2}},$$

where  $b$  is the impact parameter and  $\phi(r) = \frac{2U(r)E}{p_\infty^2 c^2}$ ,  $U(r)$ ,  $E$ ,  $p_\infty$  are the centrally symmetric continuous potential of bent planes, total energy, and particle momentum at infinity, respectively, is inapplicable for the entire range of impact parameters. Indeed, the above formula is the first nonzero term of the expansion of the classical deflection function

$$\chi(b) = \pi - 2b \int_{r_o}^\infty \frac{dr}{r \sqrt{r^2 [1 - \phi(r)] - b^2}}, \quad (1)$$

in the power series in the effective interaction potential  $\phi(r)$ . The crystal interaction potential  $U(r)$  is the sum of the potentials of individual bent planes concentrically located in the radial direction with period  $d$ . It has no singularities (i.e., is bounded in magnitude) and is localized in a narrow ring region at distances  $R - Nd < r < R$

(where the crystal thickness  $Nd \ll R$  and  $N$  is the number of planes). In this region,  $U(r) > 0$  and  $U(r) < 0$  for the positively and negatively charged scattered particles, respectively. Beyond the ring region, it vanishes rapidly. The perturbation theory in the interaction potential is obviously well applicable if the impact parameter satisfies the inequality  $b < (R - Nd)$ . In this case, the scattering area localized in the potential range is far from the turning point  $r_o$  determined from the relation  $b = r_o \sqrt{1 - \phi(r_o)}$  and the root singularity of the turning point does not contribute to integral (1). In the general case, it can be shown [7, 8] that the condition of the convergence of the power series of  $\phi$  is a monotonic increase in the function  $u(r) = r \sqrt{1 - \phi(r)}$  (e.i.  $u(r)' > 0$ ) in the  $r$  regions substantial for integral (1). Such a monotonicity is achieved if the energy and momentum of the relativistic particle satisfy the inequality

$$\frac{p_\infty^2 c^2}{2E} > U(r) + \frac{r}{2} U(r)'. \quad (2)$$

The derivation of this condition is omitted, because it was given in the Appendix in [8], but the nonrelativistic case was considered in that work. Taking into account that the inequality  $U(r) \ll r U(r)'$  is satisfied for large distances  $r \approx R$ , relation (2) is transformed to the known Tsyganov criterion [9] [ $R < \frac{p_\infty^2 c^2}{E U(r)'}]$  of the disappearance of channeling in a strongly bent crystal. Thus, the perturbation theory is obviously applicable only for strongly bent crystals, where channeling is absent. It is interesting that the nonrelativistic variant [8] of condition (2) corresponds to the criterion of the absence of the so-called spiral scattering appearing in small-energy chemical reactions [10]. For this reason, the exact solution of the problem of the relativistic scattering on the model potential of the periodic system of rectangular rings

$$U(r) = U_o \begin{cases} 1, & R - id - a < r < R - id, \\ 0, & R - (i+1)d < r < R - id - a, \\ 0, & r < R - Nd, r > R, \end{cases} \quad (3)$$

where  $i = 0, 1, \dots, (N-1)$  and  $a$  and  $d$  is the thickness of a single plane and the interplanar distance, is considered

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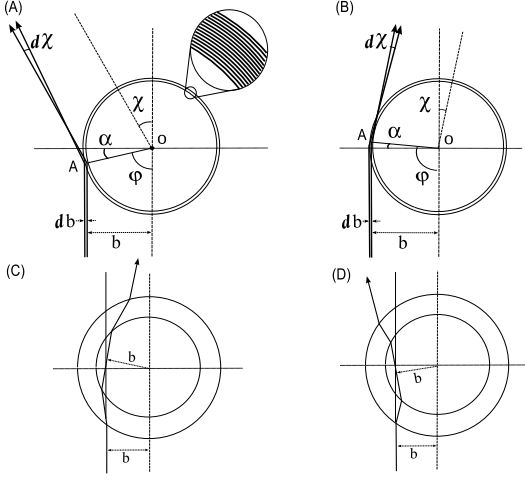


FIG. 1: Scattering of the charged particles on the ring potential: (A) reflection,  $\chi > 0$ , and (B) refraction,  $\chi < 0$ . The effect of the empty core for the (C) positively and (D) negatively charged relativistic particles.

below. With the use of the representation

$$\frac{\pi}{2} = b \int_{r_o}^{\infty} \frac{dr}{r \sqrt{r^2 [1 - \phi(r_o)] - b^2}}, \quad (4)$$

particle deflection function (1) can be rewritten in the form

$$2b \int_{r_o}^{\infty} \frac{dr}{r} \left( \frac{1}{\sqrt{r^2 [1 - \phi(r_o)] - b^2}} - \frac{1}{\sqrt{r^2 [1 - \phi(r)] - b^2}} \right). \quad (5)$$

Let us consider the range of small impact parameters,  $b < R - Nd$ , when particles penetrate into the inner region of the potential ring and twice intersect each plane. This geometry is not used in the experiments, because it requires very thin crystals. However, such an approach to solve the problem makes it possible to easily calculate the exact deflection function on potential (3) for all impact parameters and, moreover, to demonstrate an interesting property of the scattering on potentials with an empty core. This property does not seemingly attract particular attention. In this case, the turning point is located in the inner region of the potential ring, where  $\phi(r_o) = 0$ , and, as easily seen from the equation  $b = r_o \sqrt{1 - \phi(r_o)}$ , the shortest distance from the center is  $r_o = b$  (see Figs. 1C and 1D).

The deflection function for such impact parameters has the form

$$\chi(b) = 2b \int_b^{\infty} \frac{dr}{r} \left( \frac{1}{\sqrt{r^2 - b^2}} - \frac{1}{\sqrt{r^2 [1 - \phi(r)] - b^2}} \right). \quad (6)$$

Let us consider an arbitrary positive centrally symmetric potential  $\phi(r) \geq 0$ . Then, the inequality  $\frac{1}{\sqrt{r^2 - b^2}} \leq \frac{1}{\sqrt{r^2 [1 - \phi(r)] - b^2}}$  is always valid in the integrand in Eq. (6).

As immediately follows from this inequality, the scattering angles for impact parameters  $0 < b \lesssim (R - Nd)$  are always negative,  $\chi < 0$  for any form of the positive potential  $\phi(r)$ ; i.e., an arbitrary positive potential is attractive. On the contrary, an arbitrary negative potential,  $\phi(r) \leq 0$ , is repulsive. This seeming paradox is called the empty core effect. It is schematically shown in Figs. 1C and 1D and in Figs. 2A2D for the scattering on the rectangular potential and can be treated in various ways, one of which is as follows. The integral action of the positive potential deflects a particle passing through it to the left from the initial direction (see Fig. 1A); i.e., the particle is reflected. The potential in the core is absent and, according to the conservation laws, the absolute value of the momentum and angular momentum should coincide with the respective initial values. Therefore, the particle trajectory in the core should touch a circle with the radius equal to the impact parameter. This is possible only if the particle intersecting the inner boundary of the potential is deviated to the right from the initial direction. The total deflection angle is equal to the doubled angle to the turning point. Therefore, the total rotation is clockwise; i.e., the particle is attracted to the center. The opposite situation occurs for the negative potential.

Let us introduce the convenient notation

$$\Phi = 1 - \phi_o, \quad \phi_o = \frac{2U_o E}{p_o^2 c^2}, \quad \hat{r} = \frac{r}{R}, \quad \hat{b} = \frac{b}{R}, \quad \hat{a} = \frac{a}{R}, \quad (7)$$

$$\hat{d} = \frac{d}{R}, \quad \hat{b}_i = \frac{\hat{b}}{1 - i\hat{d}}, \quad \hat{b}_a = \frac{\hat{b}}{1 - \hat{a}}, \quad \hat{b}_{ia} = \frac{\hat{b}}{1 - \hat{a} - i\hat{d}}.$$

For potential (3), the scattering problem is solved exactly and deflection function (6) for  $b \lesssim R - Nd$  is represented in the form of the sum,

$$\chi(b) = 2\alpha(b) = 2 \sum_{i=0}^{N-1} \alpha_i(b), \quad (8)$$

of the integrals over the regions filled with the potential:

$$\alpha_i(b) = \hat{b} \int_{1-i\hat{d}-\hat{a}}^{1-i\hat{d}} \frac{d\hat{r}}{\hat{r}} \left( \frac{1}{\sqrt{\hat{r}^2 - \hat{b}_i^2}} - \frac{1}{\sqrt{\Phi \hat{r}^2 - \hat{b}_i^2}} \right). \quad (9)$$

Integral (9) is easily calculated and, which is most important, has an analytic continuation valid for any impact parameter:

$$\alpha_i(b) = \arcsin \left( \frac{\hat{b}_i (\sqrt{1 - \hat{b}_i^2} - \sqrt{\Phi - \hat{b}_i^2})}{\sqrt{\Phi}} \right) - \arcsin \left( \frac{\hat{b}_{ia} (\sqrt{1 - \hat{b}_{ia}^2} - \sqrt{\Phi - \hat{b}_{ia}^2})}{\sqrt{\Phi}} \right). \quad (10)$$

Note that only the real parts of the deflection function are meaningful. Therefore, if the impact parameter  $\hat{b}$  is such that any root in Eq. (10) is imaginary, it should

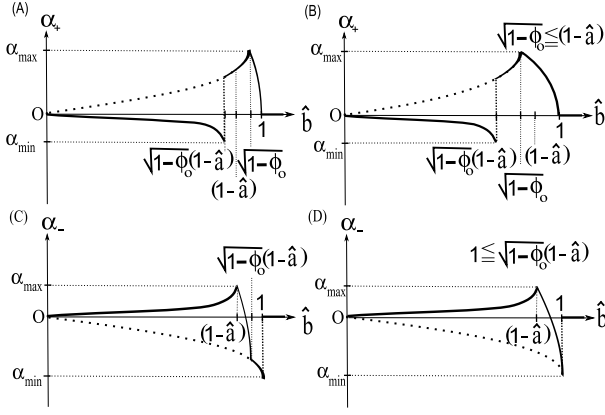


FIG. 2: Deflection function  $\alpha(\hat{b})$  for positively charged particles from the relativistic particle at (A)  $\hat{a} > \phi_o/2$  and (B)  $\hat{a} < \phi_o/2$  and for negatively charged particles at (C)  $\hat{a} > |\phi_o|/2$ , (D)-  $\hat{a} < |\phi_o|/2$ . The dotted lines correspond to the scattering on (A and B) a disc ( $U_o > 0$ ) and (C and D) a well ( $U_o < 0$ ). The region of the empty core effect for positively charged particles  $0 < \hat{b} < \sqrt{\Phi}(1 - \hat{a})$  is smaller than the inner radius  $(1 - \hat{a})$ .

be rejected. In what follows, an approximation that is not strictly necessary is used. All below formulas can be derived without this approximation, but it significantly simplifies the form and use of all of the expressions, is accepted. For small angles entering into Eq. (10) and  $\Phi \approx 1$  in the denominators in Eq. (10), Eq. (10) can be represented in the form

$$\alpha_i(b) = \hat{b}_i(\sqrt{1 - \hat{b}_i^2} - \sqrt{\Phi - \hat{b}_i^2}) - \hat{b}_{ia}(\sqrt{1 - \hat{b}_{ia}^2} - \sqrt{\Phi - \hat{b}_{ia}^2}). \quad (11)$$

Let us consider the deflection function given by Eq. (10) for one ring ( $N = 1$  and  $i = 0$ ) in more detail:

$$\alpha(b) = \arcsin\left(\frac{\hat{b}(\sqrt{1 - \hat{b}^2} - \sqrt{\Phi - \hat{b}^2})}{\sqrt{\Phi}}\right) - \arcsin\left(\frac{\hat{b}_a(\sqrt{1 - \hat{b}_a^2} - \sqrt{\Phi - \hat{b}_a^2})}{\sqrt{\Phi}}\right). \quad (12)$$

If the inner ring radius is equal to zero, then  $\hat{a} = 1$  and last two radicals in Eq. (12) become minimal. According to the above rule, they should be rejected. The resulting exact function describes the scattering of the particles on a rectangular cylindrical disc ( $U_o > 0$ ) or well ( $U_o < 0$ ) [6] (see Fig. 2).

Furthermore, let us analyze the range of impact parameters in the ring region  $(1 - N\hat{a}) \leq \hat{b} \leq 1$ , where  $\hat{b}_i$  and  $\hat{b}_{ia} \cong 1$  and can be taken due to the smallness  $N\hat{a} \ll 1$  and these factors in Eq. (11) can also be omitted. In this approximation, Eq. (12) has the form

$$\alpha(b) = (\sqrt{1 - \hat{b}^2} - \sqrt{\Phi - \hat{b}^2}) -$$

$$(\sqrt{1 - \hat{b}_a^2} - \sqrt{\Phi - \hat{b}_a^2}). \quad (13)$$

For various  $\phi_o$  values ( $\phi_o$  is the square of the Lindhard critical angle with the sign of the charge of the scattered particle), there are two sequences of critical points that can pass through the impact parameter  $\hat{b}$  when increasing from 0 to 1. For the positive potential  $U_o > 0$  ( $\Phi < 1$ ), the critical points form a sequence  $\sqrt{\Phi}(1 - \hat{a}) < \sqrt{\Phi} < 1$ . Thus, the deflection function for positively charged particles on one ring has the form

$$\alpha(\hat{b})_+ = \quad (14)$$

$$\begin{cases} (\sqrt{1 - \hat{b}^2} - \sqrt{\Phi - \hat{b}^2}) - (\sqrt{1 - \hat{b}_a^2} - \sqrt{\Phi - \hat{b}_a^2}), \\ \text{for } 0 < \hat{b} < \sqrt{\Phi}(1 - \hat{a}); \\ \sqrt{1 - \hat{b}^2} - \sqrt{\Phi - \hat{b}^2}, \text{ for } \sqrt{\Phi}(1 - \hat{a}) < \hat{b} < \sqrt{\Phi}; \\ \sqrt{1 - \hat{b}^2}, \text{ for } \sqrt{\Phi} < \hat{b} < 1; \\ 0, \text{ for } 1 < \hat{b}. \end{cases}$$

For negative potential  $U_o < 0$  ( $\Phi > 1$ ), the critical points form another sequence  $(1 - \hat{a}) < (1 - \hat{a})\sqrt{\Phi} < 1$ . It provides the deflection function for the scattering of negatively charged particles on one ring:

$$\alpha(\hat{b})_- = \quad (15)$$

$$\begin{cases} (\sqrt{1 - \hat{b}^2} - \sqrt{\Phi - \hat{b}^2}) - (\sqrt{1 - \hat{b}_a^2} - \sqrt{\Phi - \hat{b}_a^2}), \\ \text{for } 0 < \hat{b} < (1 - \hat{a}); \\ \sqrt{1 - \hat{b}^2} - \sqrt{\Phi - \hat{b}^2} + \sqrt{\Phi - \hat{b}_a^2}, \\ \text{for } (1 - \hat{a}) < \hat{b} < (1 - \hat{a})\sqrt{\Phi}; \\ \sqrt{1 - \hat{b}^2} - \sqrt{\Phi - \hat{b}^2}, \text{ for } (1 - \hat{a})\sqrt{\Phi} < \hat{b} < 1; \\ 0, \text{ for } 1 < \hat{b}. \end{cases}$$

Figures 2A and 2C show deflection functions (14) and (15), respectively, for  $|\phi_o|/2 < \hat{a}$ . If the potential is sufficiently large,  $|\phi_o|/2 > \hat{a}$ , the arc of the reflection of the positively charged particles from the outer wall of a bent plane extends to the left and can be larger than the width of the ring (and the distance between rings if the system of rings is considered). This effect causes the reflection of relativistic particles in the crystal. For negatively charged particles, when  $|\phi_o|/2 > \hat{a}$ , the corresponding reflection from the inner wall of the potential is shifted to the right and, correspondingly, the impact parameter region for the refraction of negatively charged particles is narrowed. However, at least the narrow refraction region always exists. These two variants are shown in Figs. 2B and 2D. The substitution of  $\hat{b} = \sqrt{\Phi}$ ,  $\hat{b} = \sqrt{\Phi}(1 - \hat{a})$  and  $\hat{b} = (1 - \hat{a})$ ,  $\hat{b} = 1$  into Eqs. (14) and (15), respectively, provides the maximum (minimum) deflection angles for the positively and negatively charged particles, respectively:

$$\begin{aligned} \alpha_{max+} &= -\alpha_{min-} = \sqrt{|\phi_o|}, \\ \alpha_{min+} &= -\alpha_{max-} = \frac{|\phi_o|}{2\sqrt{2\hat{a}}} - \sqrt{|\phi_o|}. \end{aligned} \quad (16)$$

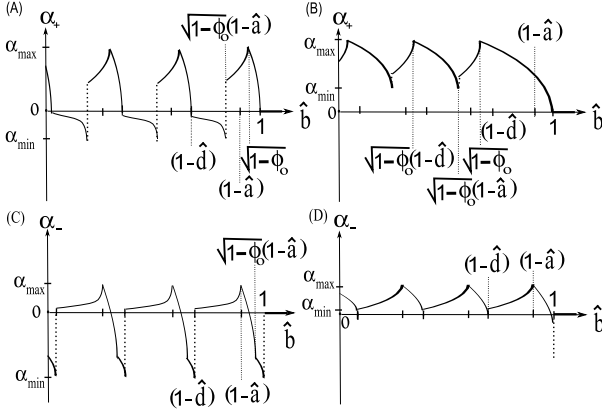


FIG. 3: Deflection function for the ring crystal and positively charged particles at (A)  $\hat{a} > \phi_o/2$  and (B)  $\hat{d} < \phi_o/2$  and for negatively charged particles at (C)  $\hat{a} > |\phi_o|/2$  and  $\hat{d} < |\phi_o|/2$ .

The deflection functions for the system of bent planes forming the crystal are similarly obtained from Eqs. (8) and (11). In this case, the summation in Eq. (8) should be performed from 0 to  $k1$ , where  $k$  is the ordinal number of the radial period containing the turning point. The sequences of the critical points mentioned before Eqs. (14) and (15) and reflection functions given by Eqs. (14) and (15) refer to the  $k$ -th period. The formulas for the reflection functions are omitted in this short paper, but the corresponding plots are presented in Fig. 3. Two length parameters,  $\hat{a}$ ,  $\hat{d}$  ( $\hat{a} < \hat{d}$ ), exist in the periodic system of bent planes. Hence, three different variants of the curves can exist with (i)  $\hat{d} > \hat{a} > \phi_o/2$ , (ii)  $\hat{d} > \phi_o/2 > \hat{a}$ , and (iii)  $\phi_o/2 > \hat{d} > \hat{a}$ . Figure 3 shows the final result for the reflection function in the first and third variants.

As mentioned above, under the condition

$$\phi_o > \frac{2d}{R}, \quad (17)$$

the refraction regions of positively charged particles disappear in the pattern of the deflection function (see Fig. 3B). Since this effect is of an applied interest for controlling the relativistic particle beams, let us calculate the average reflection angle under these conditions. For a rough estimate, the extreme ring where the deflection function has the simplest form of Eq. (14) is used. The average deflection angle in the impact parameter range  $\sqrt{\Phi} < \hat{b} < 1$  is determined by the integral

$$\bar{\alpha}_+ = \frac{1}{1 - \sqrt{\Phi}} \int_{\sqrt{\Phi}}^1 \sqrt{1 - \hat{b}^2} d\hat{b} \cong \frac{2\sqrt{\phi_o}}{3}. \quad (18)$$

Thus, the average reflection angle is  $\chi_+ = 2\bar{\alpha}_+ = 4\sqrt{\phi_o}/3$ , which is equal to  $1.33 \cdot \theta_L$ . A more accurate estimate of the reflection angle can be obtained by averaging over any inner period of the reflection function.

Let us use the second impact parameter period from the edge,  $(1 - \hat{d})\sqrt{\Phi} < \hat{b} < \sqrt{\Phi}$  (see Fig. 3B). In this case, it is unnecessary to calculate the total sum in Eq. (8); it is sufficient to calculate the reflection function at two extreme rings. This problem is solved by calculating two integrals

$$I_1 = \int_{(1-\hat{d})\sqrt{\Phi}}^{(1-\hat{a})\sqrt{\Phi}} \left( (\sqrt{1 - \hat{b}^2} - \sqrt{\Phi - \hat{b}^2}) - (\sqrt{1 - \hat{b}_a^2} - \sqrt{\Phi - \hat{b}_a^2}) + \sqrt{1 - \hat{b}_1^2} \right) d\hat{b}, \quad (19)$$

and

$$I_2 = \int_{(1-\hat{a})\sqrt{\Phi}}^{\sqrt{\Phi}} (\sqrt{1 - \hat{b}^2} - \sqrt{\Phi - \hat{b}^2}) d\hat{b}, \quad (20)$$

with subsequent expansion in small parameters  $\hat{a}$ ,  $\hat{d}$  and  $\phi_o$ . As a result, the average deflection angle  $\bar{\alpha}_+ = (I_1 + I_2)/(\hat{d}\sqrt{\Phi})$  is obtained in the form

$$\bar{\alpha}_+ = \frac{1}{3\hat{d}} \left( \phi_o^{3/2} + (2\hat{d} + \phi_o)^{3/2} + (2\hat{d} - 2\hat{a})^{3/2} - 2\sqrt{2}\hat{d}^{3/2} - (2\hat{d} - 2\hat{a} + \phi_o)^{3/2} - (2\hat{a} - 2\hat{d} + \phi_o)^{3/2} \right) \quad (21)$$

The experiment with 1-GeV protons in a  $\langle 111 \rangle$  Si crystal with a bending radius of  $R = 0.33$  m provides an average reflection angle of  $236 \pm 6.0 \mu\text{rad}$  [2]. In view of the data  $\phi_o = \theta_L^2 = 0.289 \cdot 10^{-7}$ ,  $a = 0.78 \text{ \AA}$ ,  $d = 3.136 \text{ \AA}$ , Eq. (21) provides  $\chi_+ = 2 \cdot \bar{\alpha}_+ = 318.8 \mu\text{rad}$ .

Note that rough formula (18) provides the value  $\chi_+ = 2 \cdot \bar{\alpha}_+ = 226.6 \mu\text{rad}$  that is closer to the measured value. The experiment with 70-GeV protons in a  $\langle 111 \rangle$  Si crystal with a bending radius of  $R = 1.7$  m provides an average reflection angle of  $39.5 \pm 2.0 \mu\text{rad}$ . In view of the data  $\phi_o = \theta_L^2 = 0.58 \cdot 10^{-9}$ ,  $a = 0.78 \text{ \AA}$ ,  $d = 3.136 \text{ \AA}$ , Eq. (21) provides  $\chi_+ = 37.3 \mu\text{rad}$ , which is close to the experimental value. Formula (18) provides a smaller angle of  $32.0 \mu\text{rad}$ .

For the latest CERN experiment for the reflection of 400-GeV protons [3] in a Si crystal oriented in the  $\langle 110 \rangle$  direction ( $R = 18.5$  m,  $\phi_o = \theta_L^2 = 0.1132 \cdot 10^{-9}$ ,  $a = 0.48 \text{ \AA}$ ,  $d = 1.92 \text{ \AA}$ ) and the  $\langle 111 \rangle$  direction ( $R = 11.5$  m,  $\phi_o = \theta_L^2 = 0.1008 \cdot 10^{-9}$ ,  $a = 0.78 \text{ \AA}$ ,  $d = 3.136 \text{ \AA}$ ), Eq. (21) provides  $\chi_+ = 2 \cdot \bar{\alpha}_+ = 19.0$  and  $16.0 \mu\text{rad}$ , respectively. Rough estimate (18) provides values  $14.1$  and  $13.3 \mu\text{rad}$ , which is very close to the experimental values  $13.9 \pm 0.2$  and  $13.0 \mu\text{rad}$ , for the  $\langle 110 \rangle$  and  $\langle 111 \rangle$  orientations, respectively.

Comparison of the theoretical estimates and experimental data shows that estimate formula (18) yields a smaller reflection angle over the entire range of scanned energies than that assumingly more accurate formula (21). The experimental data reported in [1, 11] are sufficiently well reproduced by formula (21), but the results

reported in [2, 3] are closer to estimate (18). This circumstance requires a more detailed analysis of the experimental conditions and the accuracy of measurements.

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